ANLYTICAL STUDY OF SINGLE MOLECULE TRANSISTOR WITH APPLICATION TO QUANTUM INTERFERENCE

Dr. Anupam Amar[1], Dr. Anuradha Amar[2], Dr. Ranjan Prasad[3]

[1] P. G. Department of Physics, B. N. M. U. Madhepura
[2] P. G. Department of Physics, Madhepura
[3] Assistant Professor, Department of Physics, S. N. S. R. K. S. College, Saharsa

ABSTRACT

In very small objects such as nanostructures and molecules, electron transport usually does not follow Ohm's law. Several effects such as energy leakage and tunneling effects are negligible in a macroscopic conductor. But as the sizes of the conductors become comparable to nanometers, these effects become dominants. In such cases a charge carrier experiences no scattering within the conductor. The overall conductance depends upon the contact between macroscopic electrodes and the nanoscale conductor. Depending on the properties of the contact, the overall transport behavior can be very different and hence understanding the nature of the contact is extremely important in the nanoscale devices. The resistive channels of nano scale size transistor starts leaking due to quantum tunneling which affects the transport of electron in nanoscale electronic devices. The transport properties of electron have been described in the conductors of nanoscale sizes.

KEYWORDS: Nanostructures, Electron Transport, Quantum Tunneling, Electronic Devices, Conductance

1. INTRODUCTION

Electrical conductance of a macroscopic object is described by the well-known Ohm's law. If G is the conductance of the conductor, L is the length and W is the width of the rectangular conductor then $G = \sigma W/L$ Here σ is the conductivity of the conductor. It is decided mainly by the charge carrier density and the mean free path. As the conductor size gets smaller, several effects that are negligible in a macroscopic conductor become increasingly important. In very small devices of nano sizes such as nanostructures and molecules the transport properties of electron does not obey Ohm's law. There are several reasons due to which Ohm's law fails at such exceedingly small scale. If the size of the conductor is smaller than the mean free path, the electron transport is not a diffusive process as described by Ohm's law rather ; it is in a ballistic conduction regime, where a charge carrier experiences no scattering within the conductor. Secondly, the contact between macroscopic electrodes and the nanoscale conductor strongly affects the overall conductance. Depending on the properties of the contact, the overall transport behavior can be very different and hence understanding the nature of the contact is extremely important. Over all, a nanoscale object has a large charge addition energy and a quantized excitation spectrum. The electron transport especially at low temperatures is strongly affected by both these factors. Studying transport behaviors of these extremely small objects is a very interesting scientific problem, and it also has many practical implications, especially to the microelectronic industry. In recent years, studying electron transport in nanoscale objects has become one of the most active fields in condensed matter physics and also it attracted huge research efforts from various other disciplines of science. To date, many nanoscale systems have been investigated, including solid-state nanostructures as well as chemical nanostructures such as carbon nanotubes and nanocrystals [1-3].The study of the transport properties of such systems reveals a number of exciting new behaviors which cannot be explained within the framework of the conventional macroscopic theory. In this study the transport properties of electron is discussed in nanoscale conductors.

2. QUANTUM INTERFERENCE

The quantum mechanical analysis of nano- scale transistor reveals the digital behavior of the single electron nano – electronic device. The resistive channels of nano scale size transistor starts leaking due to quantum tunneling [4]. This leaking begins to play an important part in the performance of nano scale transistors. There may be several aspects of this effect such as: It begins to degrade the switching ratio. Due to the increased static power dissipation the threshold swing and the operating frequency are very much affected.The performance of molecular transistors found to be improved in the case when the resistive channel contains two destructively interfering waves. When zinc-porphyrin is coupled to graphene electrodes in a three-terminal transistor to demonstrate a $>10^4$ conductance-switching ratio at 7 kHz operating frequency and stability over $>10^5$ cycles an anti-resonance interference features in conductance can be detected [5,6]. This reproduces the behavior of electron which can be explained by density functional theory calculations and trace back the high performance to the coupling between molecular orbital's and grapheme edge states. Thus the performance of nature electron transmission can be improved due to quantum nature of electron in the devices at nanoscale size. it also highlights the basis for future development of miniaturized electronics [7,8]. The quantum effects in electron transmission can be

considered in the Tunneling field-effect transistors and single-molecule transistors when they are in nanometer dimensions. When a single molecule may be used as an active channel, then it brings the benefits of synthesis with atomic precision. In this way it provides the possibility to control quantum effects through molecular design to enable high performance of miniaturized electronic devices. It also leads to complementary functionalities such as thermoelectric recovery of waste heat, multistate switching or sensing, [9,10]. Quantum interference is a characteristic quantum effect. It is found in nanoscale charge transport. It has been predicted to enhance transistor performance. However, it is difficult to create two nanoscale quantum-coherent channels in standard conductors, because scattering leads to loss of electron coherence. Consequently, the practical use of QI has been almost exclusively limited to superconducting devices to obtain extremely sensitive magnetometers. But its potential for transistors remains largely unexplored. Destructive QI (DQI) can be controlled by electrochemical gating, whereby conductance switching over two orders of magnitude has been achieved for several cycles [9,10]. However, electrochemical gating is relatively slow and incompatible with many practical applications. Graphene source and drain electrodes enable more versatile electrostatic gating and measurement of QI in single-molecule devices. Furthermore, non-trivial transmission effects resulting from the coupling between the graphene density of states with molecular orbital's can sometimes enhance the device properties [9].

3. SINGLE MOLECULAR TRANSISTOR CHARACTERISTICS

Single molecules can offer several unique properties as an electronic unit. The size is within several nanometers for most simple molecules and hence the electronic spectrum is quantized with the typical energy scale of ~ eV. They also allow self-assembly, which is very useful in fabricating electronic devices at such a small length scale. Another huge advantage is their tremendous diversity and functionality. There exist an incredibly large number of chemicals and their different chemical and electrical functions can open up many new possibilities that have never been available.

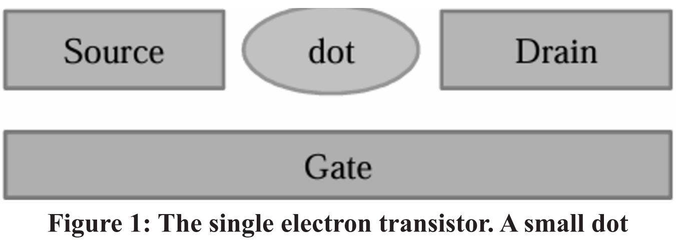

Figure 1: The single electron transistor. A small dot is separated from the source and drain electrodes by tunnel barriers. It is also coupled to the gate electrode capacitively

The theory of a single electron transistor (SET) has been explained by Kouwenhoven et al[11-13]. A very simple form of the explanation is presented here. In the figure (1) a single electron transistor has been represented schematically. Here a dot is surrounded by three electrodes. All these three electrodes are coupled to the dot capacitively. A slight change in potential in any of the capacitor can cause an electrostatic energy change in the dot. Only two electrodes, the source and the drain are tunnel coupled to the dot. The electron transport is allowed only between the dot and these two electrodes. Since the dot is connected to the source and drain electrodes by a tunnel barrier. It can be proposed that an electron is either on the dot or on one of the electrodes. Suppose that the number of electrons on the dot is N. We assume that all interactions between an electron on the dot and all other electrons on the dot or on the electrodes can be parameterized by the total capacitance C. We also assume that C does not depend on different charge states of the dot. Then the total electrostatic energy for a dot with N electrons may be written as $Q^2/2C = (Ne)^2/2C$ Where N is the number of electrons residing on the dot and e is the charge on the electron. The total energy is given as:

$U(N) = Ei + (Ne)^2/2C$, Where Ei = The chemical potential of the dot with I th electron. When an additional electron is added to the dot, the total energy becomes,

$U(N+1) = Ei + \{(N+1)e\}^2/2C$ This is the energy of the orbital of the dot that the ith electron will occupy.

The electrochemical potential is then given by:

$$\mu_N = U(N) - U(N-1) = E_N + (N-1/2)e^2$$

The electrochemical potential μ_N is defined as the minimum amount of energy required for adding the N-th electron. As long as μ_N is below both μ_S and μ_D, the N-th electron will be added to the dot. Likewise, to add one more electron to a dot with N electrons, $\mu_N+1 = \mu_N + e^2/C + \Delta E$ needs to be lower than both μS and μ D, where ΔE = EN +1 –EN.Where μ_S and μ_D are the electrochemical potentials of the source material and the drain material respectively. For simplicity, we will assume that ΔE does not change for different charge states of the dot. This allows us to drop the subscript N for ΔE. Therefore, the N+1-th electron needs to have an energy larger than the one for the N-th electron may be given by: $e^2/C + \Delta E$. This is the charge addition energy. The first term e^2/C = EC which is called the charging energy. This is the energy that is required to overcome the Coulomb repulsion among different electrons. The second term ΔE is the result of quantized excitation spectrum of the dot. These conductance peaks are called Coulomb oscillations. To be able to observe Coulomb oscillations, the charge addition energy should be much larger than the thermal energy $k_B T$. Otherwise, thermal fluctuation effect will be dominant and the Coulomb oscillation will disappear. When electric current flows through a single molecule, the conductance is mainly decided by the quantized electronic structure of the molecule. The presence of accessible charge states near the electrode Fermi levels can help electron transport through a molecule. The properties of the contact between the molecule and the leads are also important, and they strongly affect the overall conductance of a single molecule device.

4. TRANSISTOR PERFORMANCE

The optimum values of gate control that can be achieved in a field-effect transistor by the thermionic limit that results from the exponential tails of the Fermi distributions of the electrodes. But in nanodevices, its performance is usually degraded due

to presence of short-channel parasitic effects. The single-level model treats the molecular resonance as a Breit–Wigner resonance, and as it only considers transmission through a single channel, it cannot capture interference effects. The lifetime broadening and thermal broadening both contribute to the sub threshold swing in a single molecular transistor. Therefore it can be ensured that that this effect can be detected above the thermionic limit at all T, with a small change where kBT«Γ, where kB is the Boltzmann constant that becomes linear as T increases. This result reveals a fundamental trade-off when designing a three-terminal nano device for transistor applications: a larger Γ is desirable to give high on-state currents but comes at the expense of higher off-state currents and larger sub threshold swings. Even with an intermediate Γ, thereby permitting a high on-state and low off-state current that can be switched by only a small change in Vg. These observations show the value of DQI in the device performance: it effectively negates the additional contribution of lifetime broadening to the sub threshold swing, reducing the value to the thermionic limit, even in the intermediate coupling regime. The general relationship between the on/off ratio and the channel length in sub-10 nm transistors can be under stood by considering the molecule as a quantum tunneling barrier— even if the device is tuned to the off state. The devices inevitably become exponentially more transmissive with decreasing molecular length, decreasing barrier width, raising off currents and decreasing the switching ratio. Without considering the phase-coherent nature of electron transmission, this leakage current fundamentally limits the transistor performance on this length scale.

5. CONCLUSION

This study reveals that the quantum interference can be harnessed in low-power miniaturized electronic devices which are of just a few nanometers dimensions. In such devices the quantum effects are used as a resource to enhance device function. The mild fabrication method allows using a wide range of chemical compounds to create these nano scale transistors, opening the path to the creation of multifunctional devices. In the optical or spintronic properties the quantum interference can be used to control multiple effects. The overall conductance of a single molecule transistor is determined by the tunnel resistances of the contacts. In general, the contact between a molecule and the electrodes are observed to be poor and the overall conductance is significantly lower than the conductance quantum. Since there is no good control over how a molecule is contacted by electrodes. Therefore, the conductance varies from device to device even for the devices made with the same molecule.

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